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How the PHMC algorithm samples configuration space *

R. Frezzotti[a] and K. Jansen[b]

[a]Max-Planck-Institut für Physik,
Föhringer Ring 6, D-80805 München, Germany

[b]CERN,
1211 Genève, Switzerland

We show that in practical simulations of lattice QCD with two dynamical light fermion species the PHMC algorithm samples configuration space differently from the commonly used HMC algorithm.

1. Introduction

Simulations of lattice QCD with light dynamical fermions still pose severe problems, concerning both the computational cost and ergodicity properties. The PHMC algorithm [1] represents an attempt of improving on both points over the commonly used HMC algorithm [2].

The main idea [3] of the PHMC algorithm is to sample gauge configuration space -through a standard HMC method- by using an approximate action where, in the fermion sector, the inverse of the squared Hermitian Dirac operator ($Q^2 \propto M^\dagger M$) is replaced by a suitable polynomial approximant, $P_{n,\epsilon}(Q^2)$. The use of a well controlled polynomial approximation makes also possible to correct for it through an efficient reweighing technique [1], leading to exact (reweighted) sample averages for lattice QCD with $n_f = 2$ degenerate fermion species:

$$\langle \mathcal{O} \rangle = \langle W \rangle^{-1}_{PHMC} \langle \mathcal{O} W \rangle_{PHMC} \qquad (1)$$

where $\mathcal{O}$ stands for any observable and W is a noisy estimate of $\det[Q^2 P_{n,\epsilon}(Q^2)]$.

According to the Chebyshev approximation method, the polynomial in s having degree n, $P_{n,\epsilon}(s)$, approximates the function $1/s$, with $s > 0$, with a relative error that is bounded by $\delta \simeq 2\exp(-2\sqrt{\epsilon}n)$ in the range[1] $\epsilon \leq s \leq 1$ and that quickly increases as s gets smaller than ϵ. As a consequence, in the molecular dynamics (MD) update, the role of the lowest eigenvalues of Q^2, denoted here by $\lambda_{\min}$, is taken by ϵ, which can be chosen -in practice- about $2\langle \lambda_{\min} \rangle$. This leads to a computational cost per MD trajectory correspondingly smaller -by about a factor 2- than in the case of the HMC algorithm. Moreover, the approximate action used in the MD evolution makes gauge configurations with very low (compared to ϵ) eigenvalues of Q^2 to be generated with much higher probability than in the HMC algorithm. These gauge configurations are expected to be important for the sample average of many fermion observables and for associated changes of topological sectors. We then expect the PHMC algorithm to show -in critical situations- ergodicity properties that are different from the ones of the HMC algorithm.

2. Main results of PHMC tests

The PHMC algorithm has been implemented on APE computers and carefully studied [4][5]; particular care has been devoted to the role of reweighing and to the tuning of n and ϵ, for which a practical procedure was suggested [5]. All test studies were performed on lattices with Schrödinger functional (SF) boundary conditions [6], which enabled us to work at vanishing quark mass. We have used Wilson fermions -in both the standard and the O(a) improved versions- with *even–odd* preconditioning and a Sexton–Weingarten integration scheme for the MD evo-

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[1]The operator Q^2 is assumed to be normalized so that its highest eigenvalues is always smaller than 1.

Table 1
The average condition number, $\langle k \rangle$, of the preconditioned fermion matrix and the costs, $C_{Q\phi}$, of a MD trajectory in performance tests at $\kappa = \kappa_c$. More details in refs. [1] (test *a*) and [5] (tests *b*,*c*).

	Lattice	β	$c_{\rm sw}$	$\langle k \rangle$	$C_{Q\phi}^{\rm HMC}$	$C_{Q\phi}^{\rm PHMC}$
a:	8^4	5.6	0	720	7398	3974
b:	$8^3 \cdot 16$	6.8	1.4251	760	7750	5956
c:	$8^3 \cdot 16$	5.4	1.7275	1500	19734	11450

lution. Within the statistical uncertainties, we have always found consistent results for the mean values of several pure gauge and fermion observables obtained from the HMC and the PHMC algorithm.

Performance tests[2] against the HMC algorithm have been performed at *vanishing* quark mass on lattices of small and intermediate physical size, with spatial length never larger than 1 fm. This physical situation -although very different from the ones where most unquenched simulations are performed- is of practical interest for non perturbative renormalization studies. We summarize in table 1 the main results of our performance tests: the computational costs $C_{Q\phi}^{\rm HMC}$ and $C_{Q\phi}^{\rm PHMC}$ are given in units of fermion matrix (Q) times pseudo-fermion vector (ϕ) multiplications and refer to a full trajectory, accounting in the PHMC case also for the reweighing procedure. However only for tests a and b comparing these costs corresponds to a comparison of the actual costs to generate an independent gauge configuration, since for almost all the considered observables compatible errors (within O(15%) relative uncertainties) are obtained from the two algorithms when the same statistics is employed. In the case of test c the accumulated statistics is not enough to make any definite statement on statistical errors and corresponding uncertainties. Moreover a direct performance comparison is made problematic by the significant differences in sampling the configuration space that we are going to discuss.

As shown in fig. 3 of ref. [4] and fig. 4 of ref. [5], the PHMC sample in the case of test c includes a significant fraction of configurations carrying

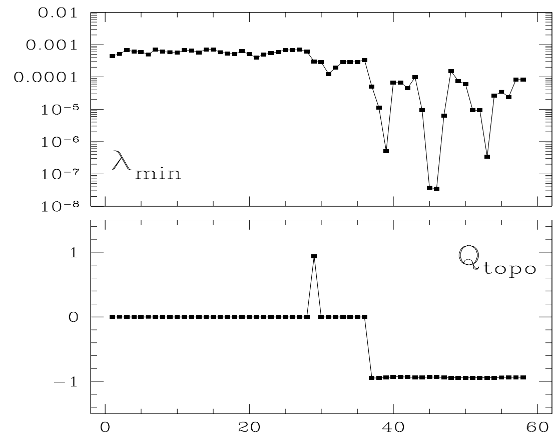

Figure 1. An example of Monte Carlo time evolution for $\lambda_{\rm min}$ and the naive topological charge after cooling, $Q_{\rm topo}$.

one (or few) isolated modes of the fermion matrix lying some orders of magnitude below the average value of $\lambda_{\rm min}$. Moreover, different values of the naive topological charge are measured after 500 cooling iterations, suggesting that changes of topological sectors do occur - even at zero quark mass and in a space volume less than 1 fm^3. A typical example is shown in fig. 1. We recall that no index theorem has to hold in this case and refer to [5] for further considerations. No exceptionally small eigenvalues were observed in the corresponding HMC simulation [7].

We present in fig. 2 the Monte Carlo time evolution of the four–fermions Green function $f_A(T/2)$ (see e.g. eq.(14) of ref. [5] for its definition), taking two typical Monte Carlo history segments from our PHMC and HMC data. In the PHMC case we see that peaks for $f_A(T/2)$ occur in coincidence with very small values of $\lambda_{\rm min}$. The contributions to QCD sample averages, eq.(1), coming from these "exceptional" configurations, are made of "normal" size by the corresponding small values of W. Many examples of this behaviour, with even larger spikes in the values of $f_A(T/2)$ and $\lambda_{\rm min}$, were seen in the PHMC data. A similar behaviour has been also observed in numerical studies of Supersymmetry [8]. On the other hand, the HMC algorithm seems to generate with very low probability these exceptional configurations, from which a relevant finite contribution to QCD sample averages for many fermion observ-

[2] We omit to discuss here many tests on 4^4 lattices [4].

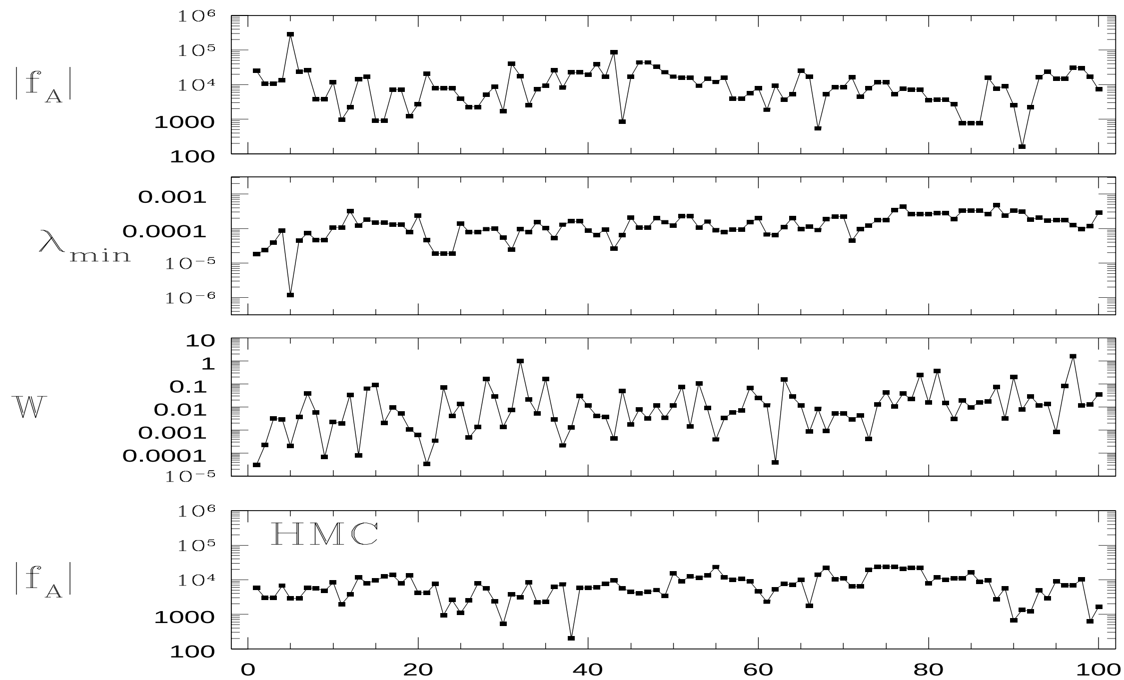

Figure 2. A segment of the Monte Carlo history of $f_A(T/2)$ as obtained from the PHMC and the HMC algorithms. In the PHMC case we also show the corresponding history of $\lambda_{\min}(\hat{Q}^2)$ and W.

ables may in principle come.

3. Conclusions

We have shown that the PHMC algorithm, as expected, samples the gauge configuration space differently from the HMC algorithm, while being at least competitive with it from the performance point of view. If gauge configurations carrying exceptionally small eigenvalues of the fermion matrix are important for some observables, the PHMC algorithm should be largely superior, owing to its ability[3] of sampling and properly treating these configurations. We think that consequences of the different ergodicity and performance properties of the HMC and the PHMC algorithm deserve to be further studied with more statistics and on larger volumes.

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[3] This remains true even in presence of exact fermion zero modes, as discussed in [4].

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